1-Methylcyclopropene

Other names: Cyclopropene, 1-methyl-
Inchi: InChI=1S/C4H6/c1-4-2-3-4/h2H,3H2,1H3
InchiKey: SHDPRTQPPWIEJG-UHFFFAOYSA-N
Formula: C4H6
SMILES: CC1=CC1
Mol. weight [g/mol]: 54.09
CAS: 3100-04-7

Physical Properties

Property code	Value	Unit	Source
affp	856.00	kJ/mol	NIST Webbook
basg	826.90	kJ/mol	NIST Webbook
chg	-2675.10 ± 1.10	kJ/mol	NIST Webbook
gf	71.59	kJ/mol	Joback Method
hf	244.00 ± 1.00	kJ/mol	NIST Webbook
hfus	4.01	kJ/mol	Joback Method
hvap	25.67	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.336		Crippen Method
mcvol	52.060	ml/mol	McGowan Method
pc	4973.33	kPa	Joback Method
rinpol	426.50		NIST Webbook
rinpol	426.50		NIST Webbook
tb	306.47	K	Joback Method
tc	488.95	K	Joback Method
tf	170.30	K	Joback Method
vc	0.203	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	69.28	J/mol×K	306.47	Joback Method
cpg	101.41	J/mol×K	458.53	Joback Method
cpg	95.79	J/mol×K	428.12	Joback Method

cpg	89.79	J/mol×K	397.71	Joback Method
cpg	83.39	J/mol×K	367.30	Joback Method
cpg	76.56	J/mol×K	336.88	Joback Method
cpg	106.67	J/mol×K	488.95	Joback Method
dvisc	0.0001785	Pa×s	306.47	Joback Method
dvisc	0.0001916	Pa×s	283.78	Joback Method
dvisc	0.0002082	Pa×s	261.08	Joback Method
dvisc	0.0002299	Pa×s	238.39	Joback Method
dvisc	0.0002593	Pa×s	215.69	Joback Method
dvisc	0.0003007	Pa×s	193.00	Joback Method
dvisc	0.0003628	Pa×s	170.30	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3100047&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

affp: Proton affinity

basg: Gas basicity

chg: Standard gas enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

pc: Critical Pressure

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume